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JMMC 2013

JOINT MEETING ON MEDICINAL CHEMISTRY



VIIIth Joint Meeting on Medicinal Chemistry, June 30-July 4 2013, Lublin

14.15-16.00 - Plenary lecture III (45')

Session moderators – prof. Armin Buschauer prof. Lucija Peterlin Mašič

PL-III

Prof. Christa Müller, University of Bonn, Germany "Purine-binding membrane proteins as drug targets"

Main lecture V-VI (30')

ML-V

Prof. Stanislav Gobec, University of Ljubljana, Slovenia "Development of new multi-target-directed ligands as potential anti-Alzheimer agents"

ML-VI

Prof. Giuseppe Ronsisvalle, University of Catania, Italy "Multitarget opioid ligands and new strategies for neuropathic pain relief"

16.00-16.30 - Coffee break

16.30-18.00 - Main lecture VII-IX (30')

Session moderators – prof. Anna Tsantili-Kakoulidou Prof. Gerhard Ecker

ML-VII

Prof. Peter Gaertner, Vienna University of Technology, Austria "Synthesis of stable isotopically labelled metabolites of doping agents and their application in analysis"

ML-VIII

Dr. Ioannis Nikolaou, Aristotle University of Thessaloniki, Greece "Bioisosterism as a useful strategy in the design of aldose reductase inhibitors (ARIs)"

ML-IX

Dr Matjaž Brvar, National Institute of Chemistry, Ljubljana, Slovenia "Discovery of novel inhibitors of DNA Gyrase B by structure-based virtual screening approach"

Tuesday, 02.07.2013

9.00-11.15 - Plenary lecture IV (45')

Session moderators – prof. Jarmila Vinšová prof. Danjiel Kikelj

PL-IV

Prof. Janusz Bujnicki, International Institute of Molecular and Cell Biology, Warsaw, Poland; Faculty of Biology, Adam Mickiewicz University, Poznan, Poland

"New computational tools for RNA 3D structure modeling, and for predicting RNA interactions with small molecule ligands"

Main lecture X (30')

ML-X

Prof. Andreas Papapetropoulos, University of Patras, Greece "Soluble guanylyl cyclase: a new look at an old drug target"

ML-VII

Synthesis of stable isotopically labelled metabolites of doping agents and their application in analysis

Peter Gaertner¹, Wolfgang Felzmann¹, Clemens Novak¹, Katharina Bica¹, Guro Forsdahl², Günter Gmeiner²

¹Institute of Applied Synthetic Chemistry, Division Organic Chemistry Vienna University of Technology, Getreidemarkt 9, A-1060 Vienna, Austria E-Mail: peter.gaertner@tuwien.ac.at

²Seibersdorf Laboratories GmbH A-2444 Seibersdorf e-mail: guenter.gmeiner@seibersdorf-laboratories.at

Partially deuterated anabolica-metabolites are especially useful as internal standards for doping analysis via GC/MS, because on one hand they have nearly identical structures and thus differences in physical and chemical properties are small, and on the other hand based on the higher molecular weight they give different molecule fragments in mass spectra and can thus be easily distinguished from the analyte which allows simple interpretation of obtained data.

To use a compound as reference it is not only necessary to have fast and easy access to this substance but also very important to provide the material in same high purity all the time.

For three selected examples, d_5 -androsteroneglucuronide (1) [1], d_5 -3´-hydroxystanozolol (2) [2], and d_5 -norandrosterone (3) [3], syntheses according to the above mentioned criteria will be presented and it will be exemplified how these compounds are used in routine doping analysis.

Literature:

- [1] P.Gaertner, C.Novak, C.Einzinger W.Felzmann, M.Knollmueller, G.Gmeiner, *Steroids* 68 (2003) 85-96
- [2] W.Felzmann, G.Gmeiner, P.Gaertner, Steroids 70 (2005) 103-110
- [3] P.Gaertner, K.Bica, W.Felzmann, G.Forsdahl, G.Gmeiner, Steroids 72 (2007) 429-436